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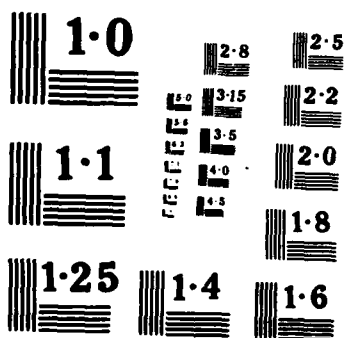
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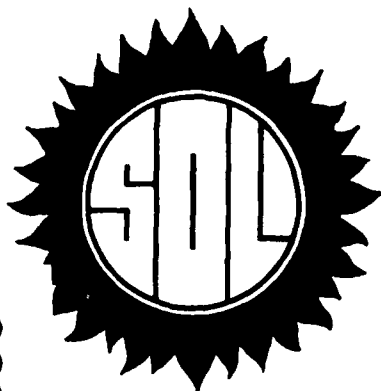
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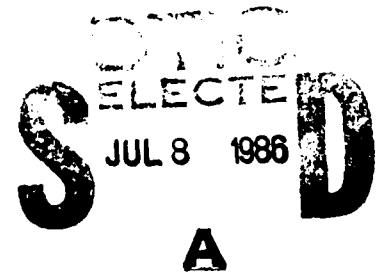
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AN ALGORITHM FOR POSITIVE DEFINITE LEAST SQUARE ESTIMATION OF PARAMETERS

Hui Hu

Abstract

We present an algorithm for positive definite least square estimation of parameters. This estimation problem arises from the PILOT dynamic macro-economic model and is equivalent to an infinite convex quadratic program. It differs from ordinary least square estimations in that the fitting matrix is required to be positive definite. The algorithm solves the infinite convex quadratic program by generating and solving a sequence of ordinary convex quadratic programs. By specifying a constant, the algorithm will find an approximate optimal solution after finitely many iterations, or will tend to an optimal solution in the limit. The algorithm is generalized to solve a class of infinite convex programs.

Key Words. Least square estimation, quadratic programming, positive definite matrix.

1. Introduction and Preliminaries

We resolve the following problem. Given two sequences of vectors a^t and b^t in R^n with $t = 1, \dots, L$, a small positive number ϵ and a large number $K \gg \epsilon$, we want to find a real symmetric matrix $X = (x_{ij})$ such that $\sum_{t=1}^L \|Xa^t - b^t\|^2$ is minimized among all the real square matrices X satisfying conditions (a) and (b):

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(a) $X^T = X$ and $-K \leq x_{ij} \leq K$ for all $i, j = 1, \dots, n$;

(b) the smallest eigenvalue of X is no less than ϵ .

This problem differs from ordinary least square estimations in that the fitting matrix X is required to be positive definite (Lemma 1). It arises from the PILOT dynamic macro-economic model designed to assess the long term impact of foreign competition, innovation, modernization and energy need (Dantzig [1]). It is a nonlinear optimization problem with matrix variables and constraints.

Throughout this paper, $S^{n-1} = \{x \in R^n: x^T x = 1\}$ denotes the unit sphere in R^n and $\| \cdot \|$ denotes the Euclidean norm. For a real symmetric matrix B , $\lambda[B]$ stands for the smallest eigenvalue of B and $v[B]$ a corresponding eigenvector of unit length. Superscripts on vectors are used to denote different vectors, while subscripts are used to denote components of a vector.

Before solving this problem, we state some lemmas about positive definite matrices and real symmetric matrices. These lemmas are either obvious or well-known; however, they play an important role throughout our discussion.

Lemma 1. For any real symmetric matrix B , the following are equivalent:

- (1) B is positive definite;
- (2) $\lambda[B]$, the smallest eigenvalue of B , is positive;
- (3) there exists $\delta > 0$ such that $u^T B u \geq \delta$ for all $u \in S^{n-1}$, where $S^{n-1} = \{x \in R^n: x^T x = 1\}$ is the unit sphere in R^n . \square

Lemma 2. For any real symmetric matrix B , $\lambda[B] = \min \{u^T B u : u \in S^{n-1}\}$ (see, e.g., Wilkinson [4], p.98-99). \square

Lemma 3. For any real symmetric matrix B , $\lambda[B]$ is a continuous function of the elements of B (see, e.g., Isaacson and Keller [3], p.136). \square

To solve this estimation problem, we first transform it into an equivalent (vector form) infinite convex quadratic program.

Given $a^t, b^t \in R^n$ for $t = 1, \dots, L$, let $A = (a^1 \dots a^L)^T$ and $B^i = (b_1^1 \dots b_1^L)^T$ for all $i = 1, \dots, n$. Let M be an $n^2 \times n^2$ block-diagonal matrix with diagonal blocks $A^T A$ and E be an $nL \times n^2$ block-diagonal matrix with diagonal blocks A . Let $X_{i\cdot}$ be the i -th row of matrix X for all $i = 1, \dots, n$ and $F(\cdot)$ be a bijection from $R^{n \times n}$ to R^{n^2} , $Y = F(X) = (X_{1\cdot} \dots X_{n\cdot})$. Then, in terms of vectors, condition (a) becomes:

$$(a) \quad Y_{(i-1)n+j} = x_{ij} = x_{ji} = Y_{(j-1)n+i} \quad \text{for all } i, j = 1, \dots, n \text{ and} \\ -K \leq Y_k \leq K \quad \text{for all } k = 1, \dots, n^2.$$

By Lemma 2, condition (b) is equivalent to: $u^T X u \geq \epsilon$ for all $u \in S^{n-1}$. Thus, condition (b) becomes:

$$(b) \quad u^T X u = \sum_{i=1}^n u_i u^T (X_{i\cdot})^T = (u_1 u^T \dots u_n u^T) Y \geq \epsilon \quad \text{for all } u \in S^{n-1}.$$

The objective function becomes:

$$\begin{aligned}
 \sum_{t=1}^L \|Xa^t - b^t\|^2 &= \sum_{t=1}^L \sum_{i=1}^n (x_{i \cdot} a^t - b_i^t)^2 \\
 &= \sum_{i=1}^n \sum_{t=1}^L (x_{i \cdot} a^t - b_i^t)^2 = \sum_{i=1}^n \|A(x_{i \cdot})^T - B^i\|^2 \\
 &= \sum_{i=1}^n \{x_{i \cdot} A^T A(x_{i \cdot})^T - 2(B^i)^T A(x_{i \cdot})^T + (B^i)^T B^i\} \\
 &= Y^T M Y - 2((B^1)^T \dots (B^n)^T) E Y + \sum_{i=1}^n (B^i)^T B^i.
 \end{aligned}$$

Consequently, the equivalent vector form optimization problem is:

$$(IQP): \text{ minimize } Y^T M Y - 2((B^1)^T \dots (B^n)^T) E Y + \sum_{i=1}^n (B^i)^T B^i$$

subject to

$$(u_1 u^T \dots u_n u^T) Y \geq \epsilon \quad \text{for all } u \in S^{n-1}$$

$$Y_{(i-1)n+j} - Y_{(j-1)n+i} = 0 \quad \text{for all } i, j = 1, \dots, n$$

$$-K \leq Y_i \leq K \quad \text{for all } i = 1, \dots, n^2.$$

Remark 1.

(1) M is positive semidefinite because each of its diagonal blocks $A^T A$ is positive semidefinite. This implies that the objective function of (IQP) is convex. The feasible region of (IQP) is compact and convex, and is defined by an infinite number of linear constraints. Moreover, it is nonempty since $\bar{Y} = F(\epsilon I)$ is a feasible solution, where I is the identity matrix. Therefore, (IQP) is a feasible infinite convex quadratic program and optimal solutions for (IQP) exist.

(2) Since $Y = F(X) = (X_1, \dots, X_n)^T$ is a bijection, $F^{-1}(\cdot)$ exists. Thus $X = F^{-1}(Y)$ and $u^T X u = u^T F^{-1}(Y) u = (u_1 u^T \dots u_n u^T) Y$. For convenience, we use $u^T F^{-1}(Y) u$ and $(u_1 u^T \dots u_n u^T) Y$ interchangeably.

We have shown that this positive definite least square estimation problem is equivalent to the infinite convex quadratic program (IQP). In Section 2, we propose an algorithm for solving (IQP) and prove its convergence. In Section 3, we present computational results for randomly generated data. Finally, we show that the algorithm presented in Section 2 can be generalized to solve a class of infinite convex programs in Section 4.

2. An Algorithm and its Convergence

We propose an algorithm for solving the infinite quadratic program (IQP). This algorithm solves (IQP) by generating and solving a sequence of feasible convex quadratic programs (QP(k)) for $k = 1, 2, \dots$. Each (QP(k)) has the same objective function as that of (IQP).

Algorithm 1

Step 1.

Let $k := 0$;

let α be a constant such that $\epsilon \leq \alpha < K$;

let (QP(k)) be the following quadratic program:

$$\text{minimize } Y^T M Y - 2((B^1)^T \dots (B^n)^T) E Y + \sum_1 (B^1)^T B^1$$

subject to

$$Y_{(i-1)n+j} - Y_{(j-1)n+i} = 0, \quad i, j = 1, \dots, n$$

$$-K \leq Y_i \leq K, \quad i = 1, \dots, n^2.$$

Step 2.

Find an optimal solution Y^k of $(QP(k))$;

let $X^k = F^{-1}(Y^k)$, i.e., $x_{ij}^k = Y_{(i-1)n+j}^k, \quad i, j = 1, \dots, n$;

calculate $\lambda[X^k]$ and $v[X^k]$;

if $\lambda[X^k] \geq \epsilon$, go to Step 4.

Step 3.

Let $u^k = v[X^k]$;

form $(QP(k+1))$ by adding a cut, $(u^k)^T F^{-1}(Y) u^k \geq \alpha$, to $(QP(k))$;

$k := k + 1$;

go to Step 2.

Step 4.

If $\alpha > \epsilon$, Y^k is an approximate optimal solution of (IQP) ; stop.

If $\alpha = \epsilon$, Y^k is an optimal solution of (IQP) ; stop.

Comments.

(1) For any k , the feasible region of $(QP(k))$ is a nonempty polytope since $Y = F(\alpha I)$ is a feasible solution. Therefore, optimal solutions exist for all $(QP(k))$. Furthermore, since the objective function of $(QP(k))$ is quadratic and convex, there are finite algorithms for finding its optimal solutions.

(2) Efficient finite algorithms for calculating eigenvalues and eigenvectors of a matrix can be found in Wilkinson [4].

(3) k counts the number of major iterations (step 2-step 3), or equivalently, the number of cuts added before termination. Each major iteration can be processed finitely.

(4) α is a constant and $\epsilon \leq \alpha < K$. If $\alpha > \epsilon$, then an approximate optimal solution will be found after a finite number of major iterations (see Theorem 1). If $\alpha = \epsilon$, then any cluster point of the sequence Y^0, Y^1, Y^2, \dots is an optimal solution for (IQP) (see Theorems 2 and 3).

Theorem 1. If $\alpha > \epsilon$, then Algorithm 1 can find an approximate optimal solution for (IQP) after a finite number of major iterations.

Proof. Let $H(Y) = Y^T M Y - 2((B^1)^T \dots (B^n)^T) E Y + \sum_1 (B^i)^T B^i$ be the objective functions of (IQP) and (QP(k)) for all k . Let $C = \{Y: -K \leq Y_i \leq K, i = 1, \dots, n^2\} \times S^{n-1}$ and $G(Y, u) = u^T F^{-1}(Y) u$. Then $G(Y, u)$ is a continuous function and C is a compact set. Hence, $G(Y, u)$ is uniformly continuous on C , i.e., for any $\delta > 0$, there exists $\eta > 0$ such that

(c) $\|(Y, u) - (\bar{Y}, \bar{u})\| < \eta$ implies $|G(Y, u) - G(\bar{Y}, \bar{u})| < \delta$ for all (Y, u) and (\bar{Y}, \bar{u}) in C .

In particular, for $\bar{\delta} = \alpha - \epsilon > 0$, there exists $\bar{\eta} > 0$ such that (c) holds. If Algorithm 1 goes on infinitely, then it generates $u^k \in S^{n-1}$ for $k = 0, 1, 2, \dots$. Since S^{n-1} is compact, for the $\bar{\eta} > 0$, there

exist u^{k_1} and u^{k_j} in the sequence such that $\|u^{k_1} - u^{k_j}\| < \bar{\eta}$.

Without loss of generality, we assume that $k_1 < k_j$. Since Algorithm 1 does not stop at iteration k_j , we have:

$$(d) \quad G(Y^{k_j}, u^{k_1}) = (u^{k_1})^T F^{-1}(Y^{k_j}) u^{k_1} \geq \alpha;$$

$$(e) \quad G(Y^{k_j}, u^{k_j}) = (u^{k_j})^T F^{-1}(Y^{k_j}) u^{k_j} < \epsilon.$$

However, (d) and (e) imply that $|G(Y^{k_j}, u^{k_1}) - G(Y^{k_j}, u^{k_j})| > \alpha - \epsilon = \bar{\delta}$

while $\|(Y^{k_j}, u^{k_1}) - (Y^{k_j}, u^{k_j})\| < \bar{\eta}$, which contradicts the uniform

continuity of $G(Y, u)$ on C . Therefore, if $\alpha > \epsilon$, then Algorithm 1

terminates finitely. Suppose that it stops at iteration k . Then

$\lambda[F^{-1}(Y^k)] \geq \epsilon$ and by Lemma 2, Y^k is a feasible solution of (IQP).

However, since $\alpha > \epsilon$, the constraints $(u^i)^T F^{-1}(Y) u^i \geq \alpha$ for $i = 0,$

$1, \dots, k-1$ may be violated by certain feasible solutions of (IQP).

We can not guarantee that $H(Y^k) \leq H(Y)$ holds for all feasible Y .

But, if $Y \in \{Y \in R^n: u^T F^{-1}(Y) u \geq \alpha \text{ for all } u \in S^{n-1}, F^{-1}(Y)^T = F^{-1}(Y),$

$-K \leq Y_i \leq K \text{ for } i = 1, \dots, n^2\}$, then $H(Y^k) \leq H(Y)$ is guaranteed to

hold. Therefore, Y^k is only an approximate optimal (or α -suboptimal)

solution in the case $\alpha > \epsilon$. \square

Remark 2. When α increases, the number of cuts added before

terminating decreases, but the final objective function value

increases. For given data and choice of α , if the algorithm does not

terminate by a specified number of iterations, we can increase α and

try again.

Theorem 2. If $\alpha = \epsilon$ and Algorithm 1 stops at a certain iteration i ,

then Y^i is an optimal solution of (IQP).

Proof. Let $H(Y) = Y^T M Y - 2((B^1)^T \dots (B^n)^T) E Y + \sum_1 (B^1)^T B^1$ be the objective functions of (IQP) and (QP(k)) for all k. If Algorithm 1 stops at a certain iteration i, then $\lambda[X^1] \geq \epsilon$. By Lemma 2, Y^1 is a feasible solution of (IQP). Next, suppose that Y is an arbitrary feasible solution of (IQP). Because $\alpha = \epsilon$, Y is feasible for all (QP(k)). In particular, Y is feasible for (QP(i)). Since Y^1 is an optimal solution of (QP(i)), we have $H(Y^1) \leq H(Y)$. Therefore, Y^1 is an optimal solution of (IQP). \square

Theorem 3. Suppose that $\alpha = \epsilon$ and that Algorithm 1 does not stop finitely. Let the sequence Y^0, Y^1, Y^2, \dots be generated by Algorithm 1. Then any cluster point is a solution for (IQP).

Proof. Let Y^k and u^k for $k = 0, 1, 2, \dots$ be generated by Algorithm 1 with $\alpha = \epsilon$. Since Y^0, Y^1, \dots are in a compact set, there exist cluster points. Let \tilde{Y} be a cluster point and without loss of generality we assume that $\lim_k Y^k = \tilde{Y}$. We claim that for any $0 < \beta < \epsilon$, there exists an integer $N(\beta)$ such that $\lambda[F^{-1}(Y^k)] \geq \beta$ for all $k \geq N(\beta)$. Let $H(Y)$, $G(Y, u)$ and C be defined as before. Since $G(Y, u)$ is uniformly continuous on C , for $\delta = \epsilon - \beta > 0$, there exists $\eta > 0$ such that

$$(f) \quad \|(Y, u) - (\tilde{Y}, \tilde{u})\| < \eta \text{ implies } |G(Y, u) - G(\tilde{Y}, \tilde{u})| < \delta \text{ for all } (Y, u) \text{ and } (\tilde{Y}, \tilde{u}) \text{ in } C.$$

Suppose that the above claim is not true. Then there exist k_i and k_j ($k_i < k_j$) such that $\lambda[F^{-1}(Y^{k_j})] < \beta$ and $\|u^{k_i} - u^{k_j}\| < \eta$. Thus,

$$(g) \quad G(Y^{kj}, u^{ki}) = (u^{ki})^T F^{-1}(Y^{kj}) u^{ki} \geq \epsilon;$$

$$(h) \quad G(Y^{kj}, u^{kj}) = (u^{kj})^T F^{-1}(Y^{kj}) u^{kj} = \lambda[F^{-1}(Y^{kj})] < \beta.$$

However, (g) and (h) imply that $|G(Y^{kj}, u^{ki}) - G(Y^{kj}, u^{kj})| > \epsilon - \beta = \delta$ while $\|(Y^{kj}, u^{ki}) - (Y^{kj}, u^{kj})\| < \eta$, which contradicts (f). Therefore, the above claim is proved. By the claim and the continuity of $F^{-1}(\cdot)$ and $\lambda[\cdot]$ (Lemma 3), we have $\lambda[F^{-1}(\tilde{Y})] \geq \beta$ for any β satisfying $0 < \beta < \epsilon$. Consequently, $\lambda[F^{-1}(\tilde{Y})] \geq \epsilon$ and \tilde{Y} is feasible for (IQP). Next, let Y be an arbitrary feasible solution of (IQP). Then Y is feasible for all (QP(k)). Because Y^k is an optimal solution of (QP(k)) and the objective functions of (QP(k)) and (IQP) are the same, we have $H(Y^k) \leq H(Y)$ for $k = 0, 1, 2, \dots$. It follows that $H(\tilde{Y}) \leq H(Y)$ holds for all feasible Y and \tilde{Y} solves (IQP). \square

Remark 3. Since $\alpha = \epsilon$, the feasible region of (QP(k)) contains that of (IQP). As the algorithm goes on, Y^k becomes more and more close to the feasible region of (IQP) and $H(Y^k)$ tends increasingly to $H(\tilde{Y})$.

3. Computational Results

We have coded Algorithm 1 in FORTRAN. We use the subroutine QPSOL (from the Systems Optimization Laboratory, Department of Operations Research, Stanford University) to solve (QP(k)) and the subroutine F02ABF (from NAG Library, Stanford University) to calculate eigenvalues and eigenvectors.

The program was executed on a DEC 20 computer. All components of the input data a^t and b^t are iid $U(-0.5, 0.5)$.

First, we compute one problem six times with different α values to demonstrate the influence of α on the number of major iterations and on the final objective values, see Table 1.

Given data:

$$L = 8, \quad \varepsilon = 1.0, \quad K = 10^9, \quad n^2 = 16;$$

$$a^1 = (-0.3052 \quad 0.1087 \quad -0.3915 \quad -0.4383)$$

$$a^2 = (0.1379 \quad 0.1707 \quad -0.1208 \quad 0.3839)$$

$$a^3 = (0.2999 \quad -0.4803 \quad 0.1790 \quad -0.2021)$$

$$a^4 = (-0.1334 \quad 0.1864 \quad -0.0431 \quad 0.4557)$$

$$a^5 = (-0.0681 \quad -0.4627 \quad -0.1384 \quad 0.0547)$$

$$a^6 = (-0.4691 \quad 0.0743 \quad 0.3823 \quad 0.1650)$$

$$a^7 = (-0.2117 \quad -0.3549 \quad 0.4991 \quad -0.1264)$$

$$a^8 = (-0.0865 \quad 0.0886 \quad -0.4886 \quad -0.3304)$$

$$b^1 = (0.2325 \quad -0.1774 \quad -0.3115 \quad 0.2133)$$

$$b^2 = (-0.4512 \quad -0.1078 \quad 0.0383 \quad -0.0906)$$

$$b^3 = (-0.0641 \quad -0.3664 \quad -0.1086 \quad -0.3182)$$

$$b^4 = (-0.3645 \quad -0.1941 \quad -0.1331 \quad -0.3830)$$

$$b^5 = (-0.2327 \quad -0.0301 \quad -0.0613 \quad 0.2470)$$

$$b^6 = (-0.3909 \quad 0.3732 \quad -0.0953 \quad -0.1953)$$

$$b^7 = (-0.1478 \quad -0.2652 \quad -0.3996 \quad 0.3307)$$

$$b^8 = (-0.2671 \quad 0.3283 \quad 0.0569 \quad -0.3668)$$

Table 1

value of α	no. of major iterations	final objective function value	CPU time (second)
1.1	4	5.2713	1.89
1.01	7	4.8017	2.77
1.001	13	4.7585	4.94
1.0001	14	4.7537	5.44
1.00001	15	4.7532	5.88
1.000001	16	4.7532	6.63

Next, we solve a number of problems in different dimensions, see Table 2. Again, all components of the input data a^t and b^t are iid $U(-0.5, 0.5)$.

Table 2

problem dimension (n^2, L)	value of α and ϵ (α, ϵ)	no. of major itera.	value of final obj. function	CPU time (second)
(16, 6)	(1.01, 1)	7	3.3775	2.90
(16, 10)	(1.01, 1)	8	5.9837	3.23
(36, 8)	(1.01, 1)	15	9.0326	25.18
(36, 12)	(1.01, 1)	17	14.1864	28.19
(64, 12)	(1.01, 1)	33	19.1114	219.29
(64, 18)	(1.01, 1)	26	29.6196	175.32

4. A Generalization

Herein we show that Algorithm 1 presented in Section 2 can be generalized to solve the following infinite convex program (ICP).

$$\begin{aligned} \text{(ICP):} \quad & \text{minimize } f(x) \\ & \text{subject to} \\ & \quad g(x,u) \geq 0 \quad \text{for all } u \in U \\ & \quad x \in S \end{aligned}$$

where U and S are compact convex sets, $f(x)$ is a convex function on S , $g(x,u)$ is continuous on $S \times U$ and is concave in x when u is fixed and convex in u when x is fixed.

Definition (ϵ -optimal solution) A vector $\bar{x} \in S$ is an ϵ -optimal solution of (ICP) if $g(\bar{x},u) \geq -\epsilon$ for all $u \in U$ and $f(\bar{x}) \leq v(\text{ICP})$, where $v(\text{ICP})$ is the optimal objective function value of (ICP).

Algorithm 2

Step 1.

Let $k := 0$;

let (CP(k)) be the following convex program:

minimize $f(x)$

subject to

$x \in S$.

Step 2.

If $(CP(k))$ is infeasible, go to Step 4;

find an optimal solution x^k of $(CP(k))$;

if $g(x^k, u) \geq 0$ for all $u \in U$, go to Step 5.

Step 3.

Find a $u^k \in U$ satisfying $g(x^k, u^k) < 0$.

form $(CP(k+1))$ by adding a cut $g(x, u^k) \geq 0$ to $(CP(k))$;

$k := k + 1$;

go to Step 2.

Step 4.

(ICP) is infeasible, stop.

Step 5.

x^k is an optimal solution of (ICP) , stop.

Notice that $g(x, u)$ is uniformly continuous on $S \times U$, it is not hard to prove the following theorems.

Theorem 4 (finite ϵ -convergence) For any $\epsilon > 0$, Algorithm 2 can find an ϵ -optimal solution of (ICP) after finitely many iterations. \square

Theorem 5 (convergence) If Algorithm 2 does not stop finitely, then any cluster point of the sequence x^k for $k = 1, 2, \dots$ is an optimal solution of (ICP) . \square

Acknowledgements. The author is very grateful to her dissertation advisor, Professor G.B. Dantzig, who suggested the problem and provided guidance throughout the research. She also would like to thank Professor A.J. Hoffman for his helpful suggestions.

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		6. PERFORMING ORG. REPORT NUMBER
7. AUTHOR(s) Hui Hu		8. CONTRACT OR GRANT NUMBER(s) N00014-85-K-0343
9. PERFORMING ORGANIZATION NAME AND ADDRESS Department of Operations Research - SOL Stanford University Stanford, CA 94305		10. PROGRAM ELEMENT, PROJECT, TASK AREA & WORK UNIT NUMBERS NR-047-064
11. CONTROLLING OFFICE NAME AND ADDRESS Office of Naval Research - Dept. of the Navy 800 N. Quincy Street Arlington, VA 22217		12. REPORT DATE May 1986
		13. NUMBER OF PAGES 15 pp.
14. MONITORING AGENCY NAME & ADDRESS (if different from Controlling Office)		15. SECURITY CLASS. (of this report) UNCLASSIFIED
		15a. DECLASSIFICATION/DOWNGRADING SCHEDULE
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18. SUPPLEMENTARY NOTES		
19. KEY WORDS (Continue on reverse side if necessary and identify by block number) least square estimation quadratic programming positive definite matrix		
20. ABSTRACT (Continue on reverse side if necessary and identify by block number) We present an algorithm for positive definite least square estimation of parameters. This estimation problem arises from the PILOT dynamic macro-economic model and is equivalent to an infinite convex quadratic program. It differs from ordinary least square estimations in that the fitting matrix is required to be positive definite. The algorithm solves the infinite convex quadratic program by generating and solving a sequence of ordinary convex quadratic programs. By specifying a constant, the algorithm will find an approximate optimal solution after finitely many iterations, or will tend to an optimal solution in the limit. The algorithm is generalized to solve a class of infinite convex programs.		

END

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